Multiscale Modeling of Fracture of Graphene Sheets and Carbon Nanotubes

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A coupling method that bridges quantum mechanical (QM) calculations, molecular mechanics (MM) simulations, and continuum mechanics (CM) was developed, and employed to simulate the fracture of defected graphene sheets and carbon nanotubes (CNTs). Different coupling strategies are used at the QM/MM and MM/CM interfaces. Coupling between MM and CM is based on a domain decomposition scheme in which displacement compatibility conditions are imposed. Coupling between QM and MM is achieved by replacing MM calculations of the energy of defect-containing fragments by direct QM simulations. The coupling method was then verified by comparing with direct QM calculations of the energetics of uniaxial tension of defected single-walled CNTs and graphene sheets. The coupling method shows a clear advantage over direct QM calculations for its computational efficiency, while offering solutions with accuracy comparable to direct QM calculations.